

Model Performance

Model

Data

Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: $1.79\text{e-}11$ cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: $3.03\text{e-}01$

Confidence level: $6.63\text{e-}01$

Nearest Neighbors from the Training Set

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Acrolein

Measured: $1.99\text{e-}11$

Predicted: $1.79\text{e-}11$

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Methacrylaldehyde

Measured: $3.35\text{e-}11$

Predicted: $3.08\text{e-}11$

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Ethene, nitro-

Measured: $1.20\text{e-}12$

Predicted: $1.70\text{e-}12$

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Vinyl fluoride

Measured: $5.56\text{e-}12$

Predicted: $5.76\text{e-}12$

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Methoxyethene

Measured: $3.35\text{e-}11$

Predicted: $3.05\text{e-}11$